Two-phase model of hydrogen transport to optimize nanoparticle catalyst loading for hydrogen evolution reaction - DTU Orbit (08/11/2017)

Two-phase model of hydrogen transport to optimize nanoparticle catalyst loading for hydrogen evolution reaction

With electrocatalysts it is important to be able to distinguish between the effects of mass transport and reaction kinetics on the performance of the catalyst. When the hydrogen evolution reaction (HER) is considered, an additional and often neglected detail of mass transport in liquid is the evolution and transport of gaseous H_2, since HER leads to the continuous formation of H_2 bubbles near the electrode. We present a numerical model that includes the transport of both gaseous and dissolved H_2, as well as mass exchange between them, and combine it with a kinetic model of HER at platinum (Pt) nanoparticle electrodes.
We study the effect of the diffusion layer thickness and H_2 dissolution rate constant on the importance of gaseous transport, and the effect of equilibrium hydrogen coverage and Pt loading on the kinetic and mass transport overpotentials. Gaseous transport becomes significant when the gas volume fraction is sufficiently high to facilitate H_2 transfer to bubbles within a distance shorter than the diffusion layer thickness. At current densities below about 40 mA/cm^2 the model reduces to an analytical approximation that has characteristics similar to the diffusion of H_2. At higher current densities the increase in the gas volume fraction makes the H_2 surface concentration nonlinear with respect to the current density. Compared to the typical diffusion layer model, our model is an extension that allows more detailed studies of reaction kinetics and mass transport in the electrolyte and the effects of gas bubbles on them.

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